

# NICKEL (Ni)

Technical Guidance Sheet Supplementary Information TGS05s, July 2012

## Contents

<b>IMPORTANT SOIL SAMPLE AND ANALYTICAL INFORMATION .....</b>	<b>3</b>
AGGREGATE SAMPLES, SOIL DEPTH AND FRACTION SIZE.....	3
TOTAL AND PARTIAL ANALYTICAL DETERMINATIONS .....	3
<b>SCALE AND USE OF NORMAL BACKGROUND CONCENTRATIONS .....</b>	<b>6</b>
USE OF VARIOGRAMS.....	6
<b>NATIONAL MAP SHOWING THE DISTRIBUTION OF NICKEL IN TOPSOILS .....</b>	<b>7</b>
<b>DESCRIPTIVE STATISTICS FOR NICKEL IN TOPSOIL DATA .....</b>	<b>9</b>
NICKEL DOMAIN PERCENTILE CLASSIFICATIONS.....	9
DESCRIPTIVE STATISTICS COPPER TOPSOIL DATA SET .....	10
DATA DISTRIBUTIONS.....	12
<b>LANDSCAPE DATA USED TO DEFINE CONTAMINANT DOMAINS.....</b>	<b>14</b>
SOIL PARENT MATERIAL .....	14
METALLIFEROUS MINING AND MINERALISATION .....	15
<b>SUMMARY OF STATISTICAL PROCEDURE TO DETERMINE NBCs .....</b>	<b>16</b>
<b>ACCESS TO DATA AND INFORMATION RESOURCES USED TO CALCULATE NBCs .....</b>	<b>19</b>
PROJECT REPORTS AND INFORMATION .....	19
PRINCIPAL CONTAMINANT DATA SETS FOR ENGLAND.....	19
SOIL PARENT MATERIAL .....	19
LAND USE DATA INCLUDING METALLIFEROUS MINING AND MINERALISATION .....	19
<b>FURTHER READING .....</b>	<b>20</b>

## List of Figures

Figure 1: Comparison of topsoil Ni concentrations in NSI samples determined by XRFS and by ICP-AES following an <i>aqua regia</i> acid digest.....	4
Figure 2: Comparison of GEMAS topsoil Ni data by analytical method and categorised by land use type.....	4
Figure 3: Comparison of topsoil As concentrations in Northern Ireland (Tellus Project) by XRFS and <i>aqua regia</i> digest ICP-MS (excluding 2 extreme outliers).....	5
Figure 4: National map of nickel distribution in topsoils with county boundaries (using G-BASE and NSI (XRFS) results) .....	7
Figure 5: Probability plot of topsoil Ni results categorised by domains.....	12
Figure 6: Boxplot of Ni topsoil results attributed to domains.....	12
Figure 7: Flow chart for the calculation of the NBC for a given contaminant domain.....	16

## List of Tables

Table 1: A summary of the nickel domain percentile classifications. Domain NBCs shown in bold red .....	9
Table 2: Descriptive statistics of underlying primary data sets for Ni in all topsoils .....	11

## Acknowledgments

This supplementary information for the nickel Technical Guidance Sheet (TGS) is compiled with information derived mainly from the reports prepared for the Department for Environment Food and Rural Affairs (Defra) soil R&D project SPI008 by the British Geological Survey. This work has been led by Chris Johnson with assistance from Louise Ander, Mark Cave and Barbara Palumbo-Roe (all BGS, Keyworth) with additional contributions and comments from Murray Lark, Barry Rawlins, Don Appleton and Chris Vane (BGS Keyworth); Stephen Lofts (CEH Lancaster); and Paul Nathaniel Land Quality Management Group, Nottingham. The authors also thank the Defra Soils Policy Team, the Project Steering Group and several Local Authority contaminated land officers who have given valuable advice to improve the content of this information sheet.

When referring to this document the following bibliographic reference should be made:

Defra, 2012. Technical Guidance Sheet on normal levels of contaminants in English soils: Nickel – supplementary information. Technical Guidance Sheet No. TGS05s, July 2012. Department for Environment, Food and Rural Affairs (Defra), Soils R&D Project SPI008. Available on-line from Defra project SPI008 [web page](#).

The nickel Technical Guidance Sheet which this document supplements:

Defra, 2012. Technical Guidance Sheet on normal levels of contaminants in English soils: Nickel. Technical Guidance Sheet No. TGS05, July 2012. Department for Environment, Food and Rural Affairs (Defra), Soils R&D Project SPI008. Available on-line from Defra project SPI008 [web page](#).

## Supplementary Information

### Important soil sample and analytical information

#### Aggregate samples, soil depth and fraction size

Both the NSI (XRFS) and G-BASE data sets are derived from a soil sample that has been aggregated (composited) from a number of subsamples collected over the area of a site, rather than a single point sample. In the case of NSI this is 25 cores (subsamples) from a 20-m square (McGrath and Loveland 1992) whereas G-BASE is 5 cores, also from a 20-m square (Johnson *et al.* 2005; Fordyce *et al.* 2005). If a sample is collected as a single core, and the result is compared to the NBC, it is important to be aware that short-range variation (which can be substantial) for the single core sample will be potentially much greater than for the samples from which the NBC values are derived (Lark, 2012).

Soil samples used to calculate the Ni NBCs have been collected from the top 15 cm of the mineral soil profile (hence they are referred to as topsoils). When the sample is collected from a site covered with vegetation the surface organic layers does not form part of the sample collected. This is important for two reasons. Firstly, any recently deposited airborne particulates that have not yet migrated into the soil profile will not be sampled and secondly, surface organic material (litter), which has the capacity to fix some contaminants from atmospheric deposition, is not included as part of the sample. In urban areas the top 15 cm will reflect historical urban land uses and in rural agricultural areas, where relevant, will be within the ploughed horizon. Surveys targeting recent airborne pollution added to the soil will generally only collect from the top 2 cm of the profile in order to bias the soil results toward the airborne pollutant inputs. Such data has not been used in the NBC calculations.

Another consideration is the soil size fraction to be submitted for chemical analysis. The <2 mm fraction is widely used for soil analyses. However, other fractions are sometimes reported (e.g. <150 µm) in order to enhance some chemical contrasts and to reduce variability in the chemical results – coarser grains mean that a single “nugget” will give rise to greater variability in the analyses than will occur with a finer more homogenous material. The NBCs calculated here are exclusively based on the <2 mm soil fraction.

#### Total and partial analytical determinations

There are established international procedures and standards for the determination of naturally occurring elements in the Earth's surface environment (Darnley *et al.* 1995). These procedures have been set up in order to develop a global database of chemical results that is compatible and of sufficient quality to be used for environmental and resource management. The analytical requirements to realise this objective includes: “*The total amount of each element present is the most fundamental (and reproducible) quantity in any sample, therefore direct measurement techniques, e.g. XRFS or neutron activation analysis (NAA), or total extraction procedures should be employed as a first priority*”. The British Geological Survey has been one of the leading organisations in the development of this global geochemical database. Therefore, the vast majority of systematically collected soil sample data that is available for NBC calculations for English soils are total element concentrations determined by XRFS. Other analytical techniques that do not give total element concentrations are used to determine the nature of occurrence and speciation of an element within a sample.

When using NBCs a common question will be “how should I interpret NBCs in the context of non-total analyses”? This was investigated as part of the data exploration phase of this project (Ander *et al.* 2012). Figure 1 shows a plot of Ni in the NSI topsoils which have been analysed by both a total (XRFS) (Rawlins *et al.*, 2012) and partial (*aqua regia* followed by ICP-AES (McGrath and Loveland, 1992). There is a linear relationship between the two analytical methods with an almost 1:1 relationship. The regression equation for NSI soils is:

$$[\text{Ni}_{\text{XRFS}}] = 0.949 + (0.878 \times [\text{Ni}_{\text{aqua regia}}]) \quad (n=3,956; R^2 = 97\%; \text{ and } P < 0.05) \dots \text{Equation 1}$$

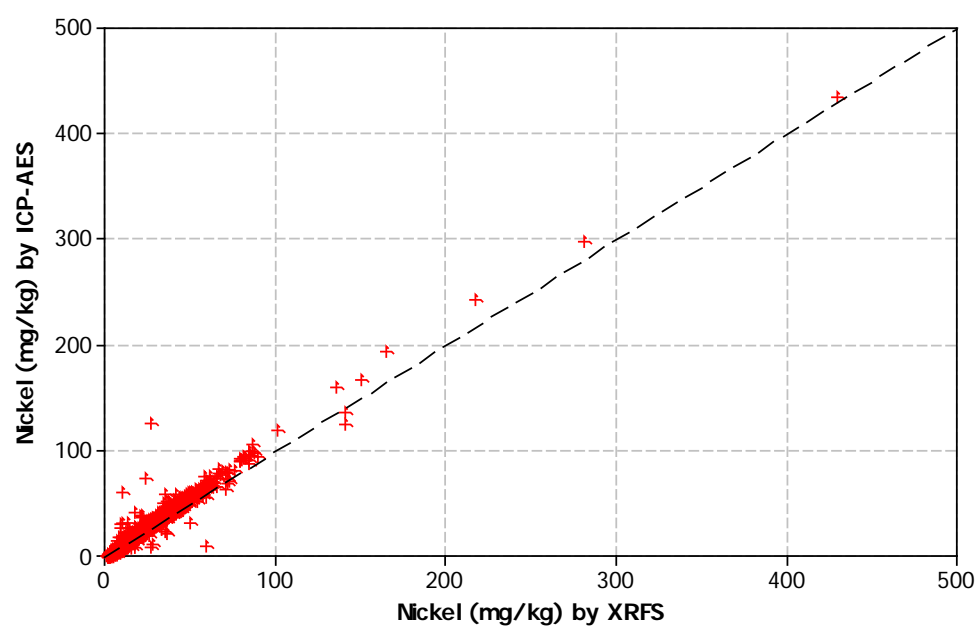


Figure 1: Comparison of topsoil Ni concentrations in NSI samples determined by XRFS and by ICP-AES following an *aqua regia* acid digest.

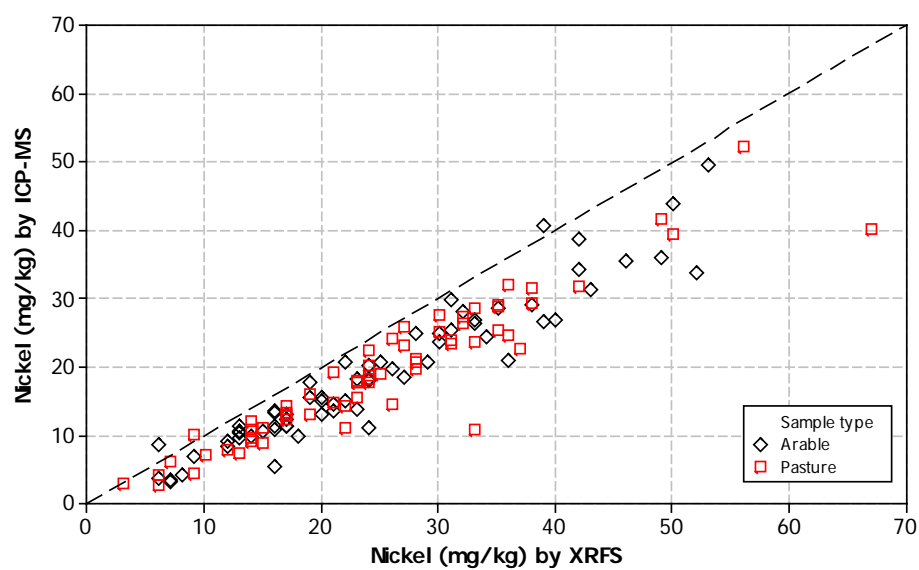


Figure 2: Comparison of GEMAS topsoil Ni data by analytical method and categorised by land use type.

## Supplementary Information

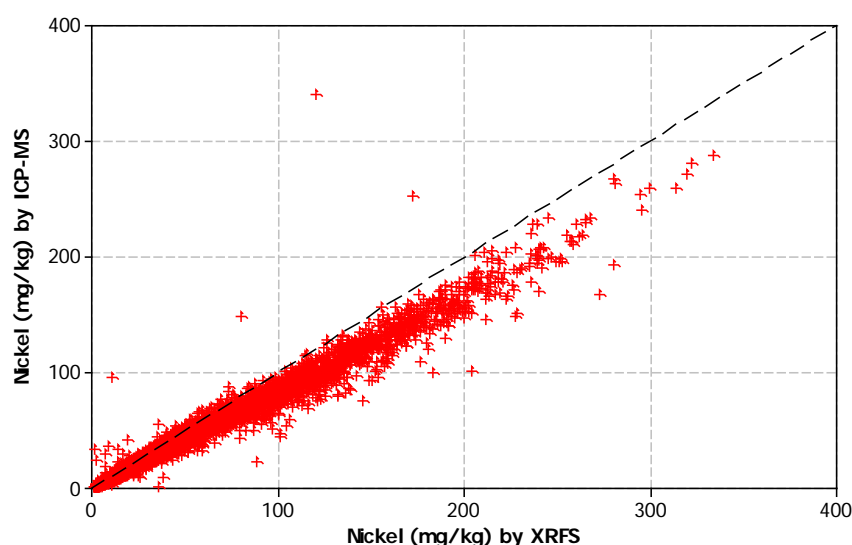


Figure 3: Comparison of topsoil As concentrations in Northern Ireland (Tellus Project) by XRFs and aqua regia digest ICP-MS (excluding 2 extreme outliers)

Similar comparisons of XRFs and ICP-MS analytical methods can be made with the GEMAS Project soils from England (Reimann *et al.*, 2012) (Figure 2) and also the Tellus Project soils from Northern Ireland (Smyth, 2007) (Figure 3). Both these data sets, as might be expected, show a systematic bias towards higher Ni results when determined by XRFs. The acid digest, unlike total measurement by XRFs, will leave a quantity of trace element-bearing, residual material. This may be greatly influenced by the type of parent material on which the soil has formed. In Northern Ireland there are a large proportion of soils developed on basic rocks (basalts). There would also be expected to be an inherent, systematic bias expected between any two analytical measurement techniques.

The regression equation for the GEMAS soil data is:

$$[Ni_{XRFs}] = 3.61 + (1.12 \times [Ni_{aqua\ regia}]) \quad (n=130; R^2 = 89\%; \text{ and } P < 0.05) \dots \text{Equation 2}$$

The regression equation for Tellus Project soil data is:

$$[Ni_{XRFs}] = 8.06 + (0.961 \times [Ni_{aqua\ regia}]) \quad (n=6,871; R^2 = 79\%; \text{ and } P < 0.05) \dots \text{Equation 3}$$

Using equations 1, 2 and 3, a soil with 50 mg/kg Ni determined by *aqua regia* followed by ICP-MS could be estimated to have a total concentration of 45, 60 and 56 mg/kg (rounded to nearest 1 mg/kg), respectively. The regression equations are therefore a tool to estimate total concentration for *aqua regia*/ICP-MS determined samples, though its application must be done with an awareness of the analytical error range, particularly at higher concentrations. The differing regression equations probably reflect slight differences in the extraction procedures and the nature of the soil's underlying parent material. The large number of samples and the diverse range of underlying parent materials would probably make the Tellus soil data (equation 3) the most reliable to base total estimates on.

### Scale and use of Normal Background Concentrations

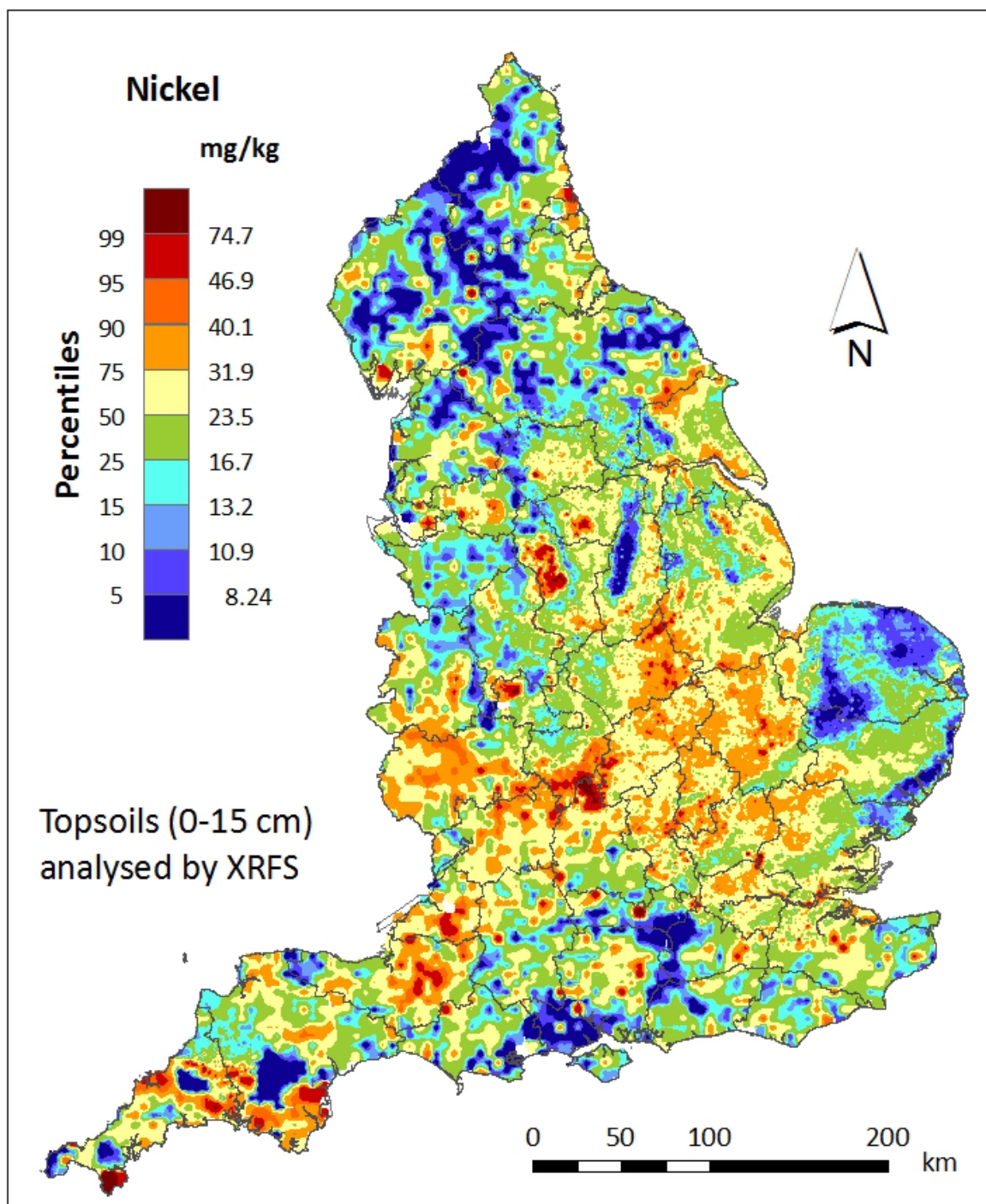
NBCs have been determined for Ni using soils collected at a range of sampling densities, from 1 sample per 0.25 km<sup>2</sup> (G-BASE urban) through to 1 sample per 25 km<sup>2</sup> (NSI XRFs). The G-BASE urban samples provide a definition of the chemical surface environment to a much higher resolution than do the NSI (XRFs) samples. Thus G-BASE rural samples (collected at 1 per 2 km<sup>2</sup> sampling density) can show contaminant variability at a local area scale (1:50,000). When investigating a sample result in the context of a NBC, it is important to ask whether localised variability (scales at less than 1:50,000), say within the Principal Domain, has been truly captured during the determination of the NBCs. Areas characterised by the lower density NSI samples are likely to miss the relatively smaller areas of basic/ultrabasic rocks (e.g. basic dykes in northern England). Therefore, a high contaminant result should be attributed to a domain, taking account of the localised underlying parent material feature, even where this has an extent which is very discontinuous.

### Use of variograms

The domains that are defined for a particular contaminant correspond to major sources of variation in concentrations of that contaminant in soil, such as urbanisation, mining or mineralisation. Concentrations of the contaminant vary within the domains, the procedure to define normal background concentrations (NBCs) quantifies this variation with robust statistics, from which the NBCs are computed. The spatial variation of a contaminant within a domain can be quantified by the variogram (Matheron, 1962). The variogram is a function that shows how the variation between observations of a variable at two sites depends on the distance in space between the sites. The variogram is half the mean squared difference between two observations plotted against the distance between them for all the results in a data set. Typically the variogram increases with distance until a plateau in the plot is reached at a value called the sill variance, which it reaches at a distance called the range. If the range is very short then this shows that the spatial variation is very intricate. If the range is longer then it may be feasible to map spatial variations from sample observations on a grid.

Supplementary Information

National map showing the distribution of nickel in topsoils



*Distribution of samples used in this interpolated map is shown in Figure 1 of the Ni technical guidance sheet.*

Figure 4: National map of nickel distribution in topsoils with county boundaries (using G-BASE and NSI (XRFS) results).

The national map of Ni distribution in topsoils (Figure 4) is shown here along with county boundaries to help with location at a regional scale. This map is given to demonstrate the variability in Ni across England and is also available to view on-line at the [BGS project web page](#). The map has been generated from G-BASE and NSI (XRFS) topsoil data using 42,133 samples. Because central and eastern England have been sampled at a much higher density (by G-BASE), resolution of information in these areas is much higher. Figure 4 has been produced in ArcGIS v9.3 using the IDW option of the Spatial Analyst tool, cell size 1000 m and search radius 5000 m (inverse square option selected). The percentile classification is based on **all data** and differs from the domain data sets in which results are modelled to fit a normal distribution and the effect of outliers (representing point rather than diffuse pollution) have been reduced by normalisation of the data.

The map shown in Figure 4 uses soils to represent the geochemical baseline. Other national/regional scale geochemical atlases for soils are those of McGrath and Loveland (1992) (NSI *aqua regia* data) and Rawlins *et al.* (2012) (NSI XRFS data). A preferred way of representing the geochemical baseline at a national/regional scale is to use stream sediments. The fine stream sediment in a drainage channel is representative of material washed down the drainage catchment to the sampling site in the stream and so gives a much better regional average of the chemical environment than is given by soils. The G-BASE project also collects stream sediments at a sampling density of approximately one sample per 2 km<sup>2</sup> and results for England have been presented in a series of atlases (e.g. Lake District (BGS 1992) and NE England (BGS 1996)) and these can be used to further demonstrate element variability across the surface environment of England. For the more recently sampled parts of England, the G-BASE project has also determined a large range of elements in stream waters (e.g. [Environmental Geochemical Atlas of Central and Eastern England](#)). Comparing the element concentrations and distributions of different sample types collected from the same locality can provide useful information about the mobility of a chemical element in that area.

A stream sediment atlas for England and Wales was also completed by Webb *et al.* (1978) (Wolfson Geochemical Atlas) and more recently low density sampling has produced continental scale geochemical baselines for Europe based on a number of sampling media, including stream sediments, stream waters and soils (Salminen *et al.* 2005) and the ongoing GEMAS project (Reimann *et al.* 2012). Appleton *et al.* (2008) using the BGS soil and stream sediment results and the Wolfson data, have produced national-scale estimation of potentially harmful element ambient background concentrations in topsoil using a parent material classified soil:stream-sediment relationships. These geochemical data have been used to derive [geospatial data sets](#) that identify the estimated concentrations (mg/kg) of As, Cd, Cr, Ni and Pb in soils.



# Technical Guidance Sheet (TGS) on normal levels of contaminants in English soils

## Supplementary Information

### Descriptive statistics for nickel in topsoil data

#### Nickel Domain percentile classifications

Percentile	Ironstone (Ni) Domain (117)			Peak District Domain (221)			Principal Domain (41,768)		
	lower	middle	upper	lower	middle	upper	lower	middle	upper
50	57	65	73	32	36	39	23	23	24
55	63	71	79	35	39	42	25	25	25
60	69	77	86	38	42	46	26	26	26
65	75	84	93	41	46	50	27	28	28
70	82	93	100	45	50	55	29	29	30
75	91	100	110	49	55	61	31	31	31
80	100	110	130	54	61	69	32	33	33
85	110	130	150	61	70	79	35	35	35
90	130	150	170	71	82	93	37	38	38
95	170	200	<b>230</b>	88	100	<b>120</b>	41	42	<b>42</b>
Percentile	Basic Domain (23)			Ultrabasic Domain (4)					
	lower	middle	upper	lower	middle	upper			
50	50	61	71	71	213	356			
55	54	64	74	78	236	372			
60	57	67	77	84	259	392			
65	60	71	81	91	282	412			
70	63	74	84	99	307	434			
75	66	78	88	107	334	458			
80	70	82	92	116	364	484			
85	74	87	97	126	399	514			
90	80	93	104	139	443	553			
95	87	103	<b>114</b>	158	508	<b>612</b>			

Figure in brackets represents the number of samples used in the domain calculation

Table 1: A summary of the nickel domain percentile classifications. Domain NBCs shown in bold red. Concentrations in mg/kg. Note that as the Ultrabasic and Basic Domain NBCs are based on less than 30 samples these values have not been used.

A percentile of a data distribution (in this case the distribution of Ni in soil for a given domain) is the value of a variable below which a certain percentage of observations fall. The 95<sup>th</sup> percentile, for example, is the value below which 95% of the observations may be found, i.e. it encompasses the majority of the data. The contaminant concentrations in the soil for a given domain are a subset of the total population of all possible soil concentrations and therefore any percentile calculation will only be an approximation of the true value. The uncertainty on the percentile increases as the number of samples used to calculate it decreases. Lower and upper limits can be statistically estimated for each percentile giving a confidence interval for that

percentile. **The Ni NBC for each domain is defined as the upper 95% confidence limit of the 95<sup>th</sup> percentile for the Ni topsoil results that fall within that domain.** A summary of domain percentiles with their upper and lower limits is given in Table 1. The domains for basic and ultrabasic rocks are shown here even though the number of samples available for their determination is below 30 (see Cave *et al.* 2012). These soil parent materials are known to be the cause of elevated Ni levels in soils (see the Tellus Project soils of Northern Ireland for example, Ander *et al.* In Press) and the NBCs can be improved as more data becomes available in England.

#### Descriptive statistics copper topsoil data set

Table 2 shows descriptive statistics for all the topsoil Ni results from the G-BASE and NSI (XRFS) data sets. The cities and towns in Table 2(c) are those that have been systematically sampled by the G-BASE project. Some of these data sets have associated reports that can be downloaded by clicking on the location place marker on the map at <http://www.bgs.ac.uk/gbase/urban.html>. Other data sets for other English cities may exist but they are not made publicly available and are not sampled and analysed to a nationally consistent standard.

# Technical Guidance Sheet (TGS) on normal levels of contaminants in English soils

## Supplementary Information

(a) All data	Number	Mean	Minimum	25th percentile	Median	75th percentile	Maximum	Skewness
G-BASE(urban + rural) + NSI (XRFS)	42133	25.6	1	16.7	23.5	31.9	506	6
(b) Data set type	Number	Mean	Minimum	25th percentile	Median	75th percentile	Maximum	Skewness
All NSI(XRFS)	4864	22.8	1.56	13.5	20.8	29.5	430	8
G-BASE (rural)	23686	24.6	1	15.6	22.6	31.5	431	4
G-BASE (urban)	13583	28.3	2.24	19.5	25.6	33.3	506	7
Eastern England (G-BASE)	23222	24.6	1	15.7	22.8	31.5	431	4
Tamar catchment (G-BASE)	464	25.3	2.61	14.5	19.3	30.7	127	2
(c) Urban (G-BASE)	Number	Mean	Minimum	25th percentile	Median	75th percentile	Maximum	Skewness
Corby	133	31.5	16.4	27.1	30.5	35.2	63.5	1
Coventry	390	24.9	6.81	17.8	23.3	29.7	157	5
Derby	275	34.1	12.5	24.6	31.3	40.6	180	4
Doncaster	279	22.1	5.9	12.3	18.7	25.1	150	4
Hull	407	34	7.73	25.1	32.4	39.7	130	2
Leicester	652	28.2	10.2	21.5	26.2	33.7	87.3	1
Lincoln	215	15.4	3.15	8.64	14.1	18.7	93.7	3
London (GLA area)	6494	28	2.28	19.7	25.5	32.7	506	8
Manchester (part of)	300	32	5.44	22.4	28.2	36.6	137	3
Mansfield	257	18.5	4.98	9.55	16	24.6	94.6	2
Northampton	275	29.9	6.26	22.4	28.1	35.2	76.7	1
Nottingham	636	28.6	5.9	19.6	26	34.2	146	3
Peterborough	272	29.9	14.3	23.6	28.2	33.8	64.5	1
Scunthorpe	196	20.4	2.24	8.64	15	26	186	4
Sheffield	575	37.7	8.64	23.3	30.6	39.7	434	6
South Essex Towns	715	27.1	5.01	18.1	24.7	31.9	210	5
Stoke-on-Trent	745	26.1	5.9	16.9	22.4	32.4	115	2
Telford	292	31.4	7.73	20.5	26.9	36.1	141	3
Wolverhampton	284	39.3	12.3	25.1	32	43.4	243	4
York	191	20.5	6.81	14.1	18.7	24.2	78.1	3

Table 2: Descriptive statistics of underlying primary data sets for Ni in all topsoils. These are classified by various data set subgroups (total concentrations (XRFS) in mg/kg) (from Ander et al. 2012, with results cited to three significant figures).

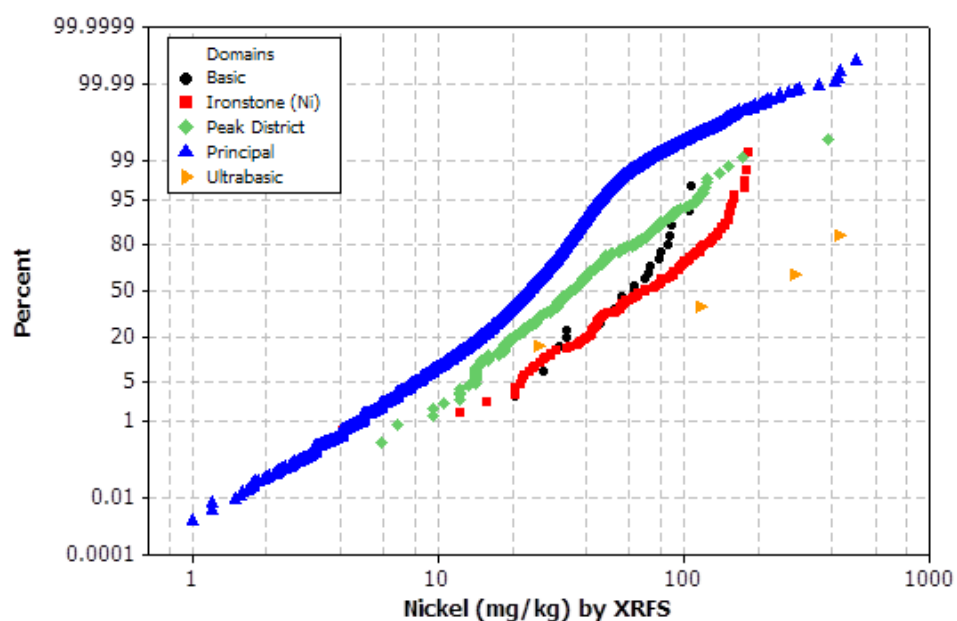


Figure 5: Probability plot of topsoil Ni results categorised by domains.

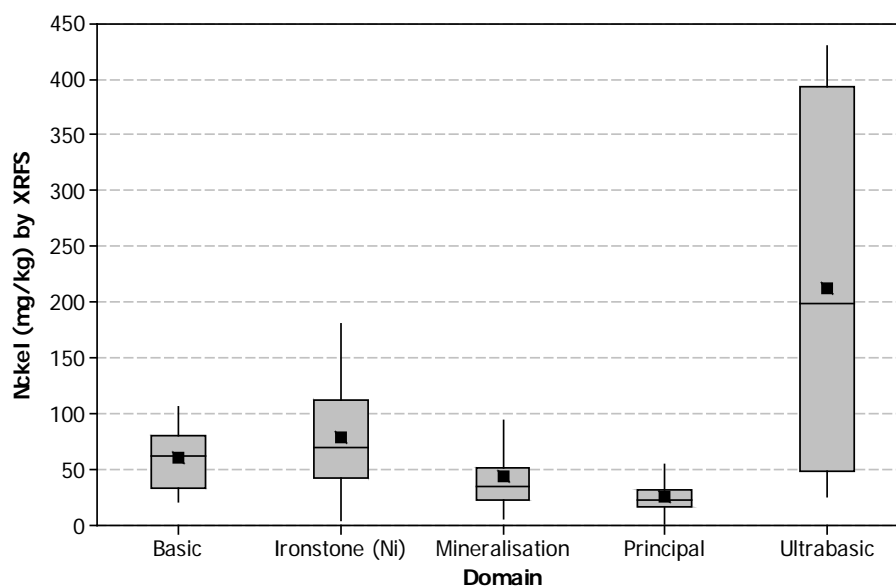


Figure 6: Boxplot of Ni topsoil results attributed to domains.

Figure 5 and Figure 6 show the frequency distribution of results for soils over the five domains defined for Ni using the G-BASE urban and rural data sets and the NSI(XRFs) data. These plots can be used in conjunction with any new results plotted in a similar way to compare distributions with the defined domains. The box of the boxplot represents the interquartile range (Q1, Q3), with the median (Q2) as a line within the box. The

### Supplementary Information

point symbol shows the mean value. The upper whisker =  $Q3 + 1.5(Q3 - Q1)$ ; lower whisker =  $Q1 - 1.5(Q3 - Q1)$ .

Archer and Hodgson (1987) carried out a study of total and extractable trace element contents of agricultural soils (from a depth of 15 cm) in England and Wales, including Ni. “Total” Ni analyses were done by AAS following a digestion using perchloric and nitric acids. They defined the normal range for trace element contents as that between twice the log-derived standard deviation above and below the mean; approximately 95% of the data range. For 1,521 agricultural topsoils they determined a Ni median of 23.7 mg/kg and a “normal” range of 7.3-70 mg/kg.

Paterson *et al.* (2003) reporting on background levels of contaminants in Scottish soils report a range of Ni concentrations for mineral soils from 0.4 – 233 mg/kg with  $Q1$ ,  $Q2$  and  $Q3$  values of 10, 17.5 and 25.7 mg/kg, respectively. These are lower than the English soils (all data - Table 2) of 16.7, 23.5 and 31.9 mg/kg ( $Q1$ ,  $Q2$  and  $Q3$ , respectively), probably reflecting the greater variety of land uses (i.e. possible anthropogenic input) associated with the English soils.

## Landscape data used to define contaminant domains

Rather than seeking to define a single Ni NBC for the whole of England, the project has, through its data exploration (Ander *et al.* 2012), determined the most significant domains that can be defined in order to capture the most significant controls on Ni distribution in soils. For Ni five domains have been identified and these (with the exception of the Principal Domain) are related to soil forming parent materials and mineralisation. Although there is evidence of some urban areas having elevated soil Ni concentrations (see Table 2c), urbanisation and industrialisation is not considered to be as significant in contributing to the “widespread and normal” Ni concentrations as is observed for other contaminants. These domains have been defined using some key datasets within a GIS environment, namely: the BGS Soil-Parent Material Model (SPMM) (Lawley, 2009) and a revised and digitally updated version of the Ove Arup (1990) Department of the Environment (DoE) Metalliferous Mining and Mineralisation data set.

### Soil parent material

The Soil-Parent Material Model<sup>1</sup> (SPMM) has been developed by BGS, using as its basis the mapped boundaries of the national 1:50,000 superficial and bedrock geological data (DigMapGB-50<sup>2</sup>), and is used within a GIS environment. Soil ‘Parent Material’ is the first recognisably geological material found beneath a soil profile, and is the lithology on which that soil has developed. Soils thus inherit many properties, including chemical composition, from this material.

In the SPMM the geological data have been combined into one layer of information which indicates the rock/sediment formation mapped as directly underlying soil. Where this is a superficial deposit (such as alluvium, glacial deposits, peat), the data set also maintains the record of the solid geological formation first encountered beneath this surface sediment; such information is of benefit where the underlying solid geology imparts chemical (or other) characteristics into the overlying superficial deposits, and thus the soil. The information, which has historically routinely been attributed to the mapped digital polygons in DigMapGB, largely comprises lithological and chronological information. Augmenting this in the SPMM is additional information on texture, mineralogy and lithology, which is attributed in a hierarchical classification system. In the context of the present study this means that a higher level of aggregated characteristics can easily be applied to soil geochemical data than is possible solely using DigMapGB; for instance, retrieving all formations which are classed as ‘ironstones’ (irrespective of their formal name) and confers benefits from using the SPMM.

The scale of mapping for the soil parent material is also relevant – 1:50,000 is the scale at which much of the systematic soil sampling has been undertaken, and gives the user a reasonable feel for the degree of uncertainty on the data. Where geographical information is provided at other common scales, such as 1:250,000 or 1:625,000, the boundaries and number of polygons are simplified and aggregated in order to provide generalised information at the national-scale. More detailed mapping, such as 1:10,000, is not available in a consistent format or as part of the SPMM data, and would imply greater certainty in sample locations and polygon boundaries than is appropriate from the data. Soil mapping is available at a national-scale (see e.g. NSRI NATMAP<sup>3</sup>) but this is not systematically mapped at 1:50,000 and would require attribution with the latest geological mapping data in order to retrieve information on key formations, and so has not been used in this study.

---

<sup>1</sup> <http://www.bgs.ac.uk/products/onshore/soilPMM.html>

<sup>2</sup> [http://www.bgs.ac.uk/products/digitalmaps/digmapgb\\_50.html](http://www.bgs.ac.uk/products/digitalmaps/digmapgb_50.html)

<sup>3</sup> <http://www.landis.org.uk/data/natmap.cfm>

### Supplementary Information

#### Metalliferous mining and mineralisation

The data set which has been examined in this project is that of non-ferrous Metalliferous Mineralisation and Mining database, originally produced in hard-copy by Ove Arup (1990) for DoE (Department of Environment), but which has been 'cleaned' and turned into a polygon layer by BGS. The data for England has been further attributed for this project by giving a name to the major ore fields allowing soil sample sites and geochemical data to be joined to the ore fields and separately analysed for typical soil concentrations. This mapping is generalised to 0.5 km grid squares, which is a suitable level of spatial resolution for this type of data.

Therefore, it should be expected that not every occurrence of mineralisation/mining has been captured within this GIS layer. Where soil chemical data is encountered that is located outside a given mineralisation domain, but of a concentration expected for that contaminant within the local mineralisation domain, and lies over the parent material which is known to be affected by mineralisation in that ore field, then that high soil concentration could relate to either natural processes, or historical mining.

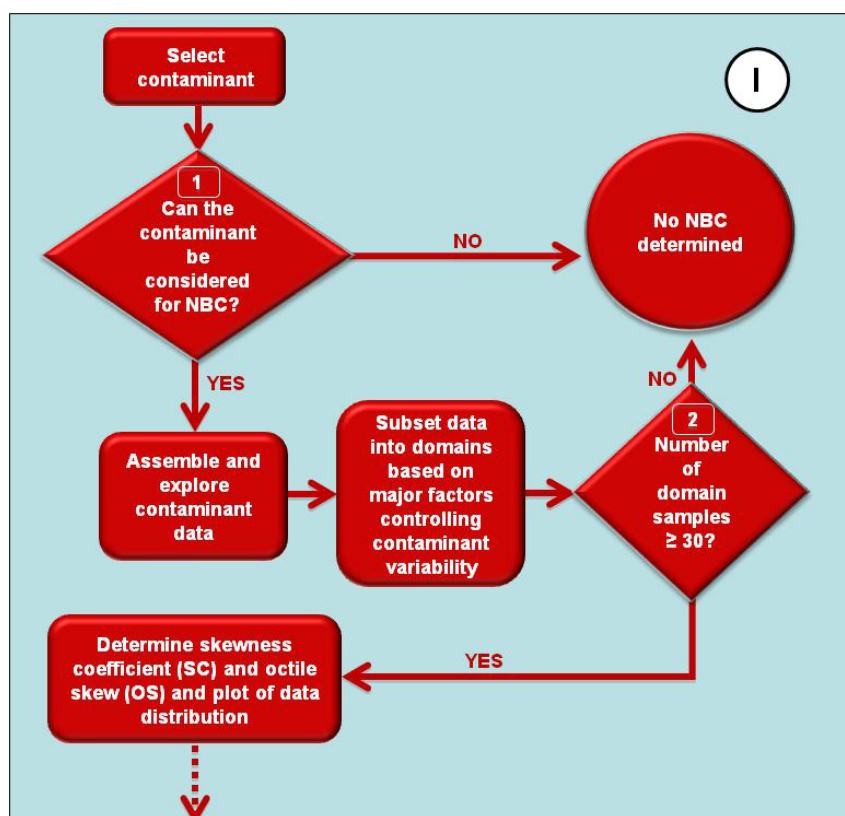


Figure 7: Flow chart for the calculation of the NBC for a given contaminant domain (OS and SC are octile skew and skewness coefficient, respectively. MAD = median absolute deviation). See text for explanation, continued overleaf.



## Supplementary Information

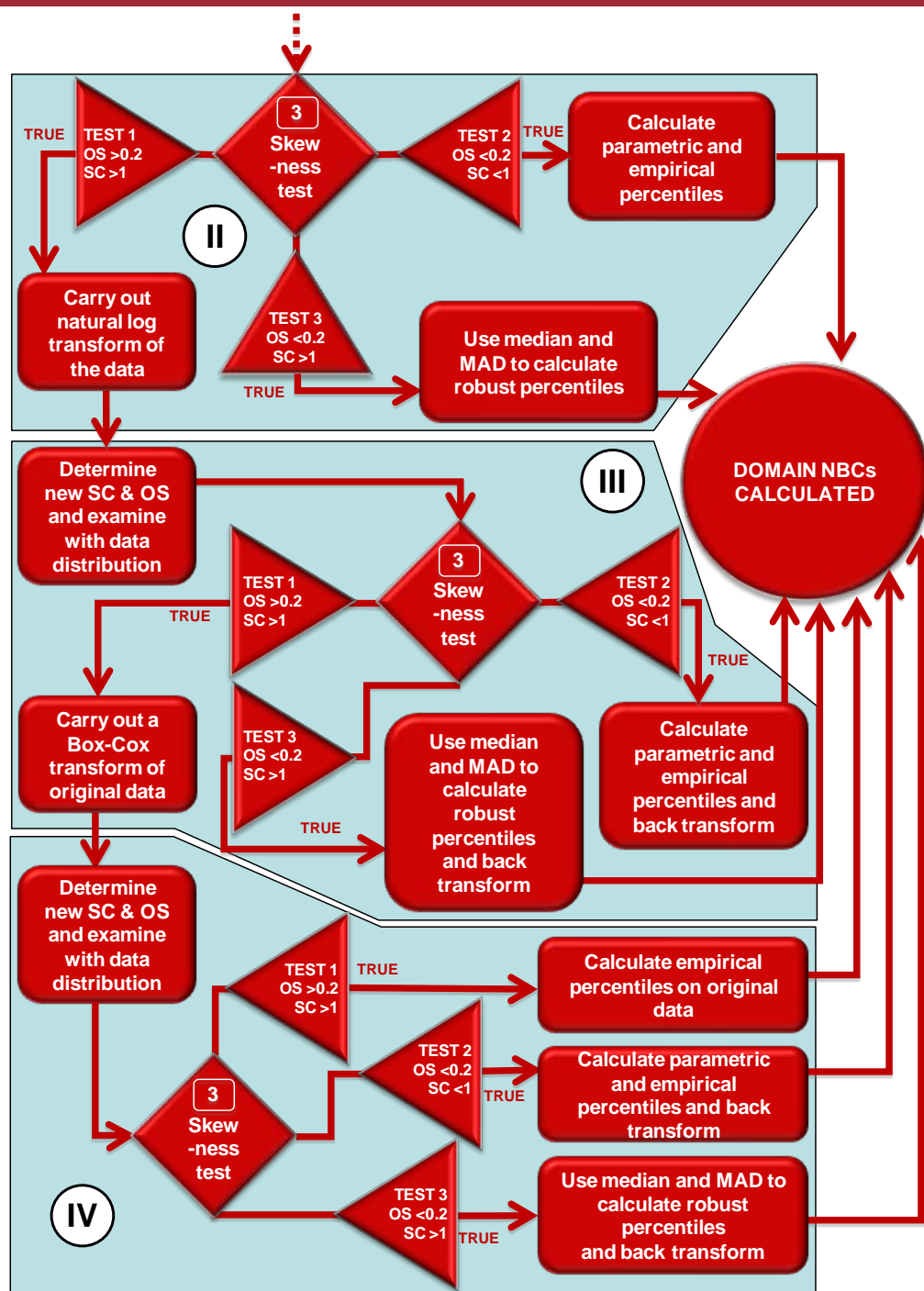


Figure 7 continued. Flow chart for the calculation of the NBC for a given contaminant domain (OS and SC are octile skew and skewness coefficient, respectively. MAD = median absolute deviation). See text for explanation.

Figure 7 summarise the statistical procedure used to determine contaminant NBCs (see Cave *et al.* 2012). Part I essentially represents the data gathering and exploration phase of the project (WPI&2) in which domain

areas are identified. Question 1 asks if the contaminant is suitable for a NBC. Asbestos and manufactured organic contaminants with no natural origin, for example, fail this question. The data exploration (Ander *et al.*, 2011) identifies the areas (domains) where there are clearly identifiable controls on high concentrations of a specified contaminant. The contaminant data set is then subdivided into domain data sets. In question 2 a minimum of 30 results are considered necessary to determine a NBC (see Cave *et al.*, 2012). Once the data has been subsetted into domains, then skewness testing and inspection of frequency distribution plots can be done to select the appropriate data transform and method of calculating percentiles (Parts II – IV). Question 3, the skewness test, has three possible outcomes. TEST 1 ( $OS > 0.2$  and  $SC > 1$ ) is true if the data distribution is skewed and not suitable for fitting to a Gaussian model and the data need to be transformed to using either a logarithmic or Box-Cox transform. If TEST 2 ( $OS < 0.2$  and  $SC < 1$ ) is true then the data are consistent with the assumption of a Gaussian distribution and the parametric percentiles are fitted based on the mean and standard deviation of the data. Finally, TEST 3 ( $OS < 0.2$  and  $SC > 1$ ) means the data show a mostly symmetrical distribution but with potential outliers. Here the data are consistent with the assumption of a Gaussian distribution and the parametric percentiles are fitted using median and the median absolute deviation (MAD) in place of the mean and standard deviation as these measures are robust to outliers.

### Supplementary Information

#### Access to data and information resources used to calculate NBCs

##### Project Reports and information

These resources are available from the [BGS project web page](#)<sup>4</sup> and include:

Data Exploration Reports (BGS report No. CR/11/145 and CR/012/041); Methodology Report (BGS report No. CR/12/003); Final Project Report (BGS report No. CR/12/035); Technical Guidance Sheets and supplementary information; MS Access Database summary of available data; Project Bibliography (Endnote bibliography); R code scripts used to determine NBCs; and GIS Resources served as WMS files (Domain polygons; the urbanisation index polygons defined from GLUD database; and the national contaminant interpolated image maps).

Web map services (WMS) are an industry standard protocol for serving georeferenced images across the web. They were developed and first published by the Open Geospatial Consortium (OGC) in 2000. Since this date WMS have had a steady uptake and are being increasingly used in traditional desktop based GIS, web-based GIS systems (including Google Earth), and Smartphone 'apps'. BGS holds the data on their servers and publish it openly via the [BGS project web page](#).

##### Principal contaminant data sets for England

Intellectual Property Rights for the raw soil data sets resides with the organisations responsible for those data sets. In the case of the G-BASE and NSI (XRFS) data is made freely available subject to certain licensing terms and conditions. For large data sets there will also be a data handling fee. Further information regarding access to the G-BASE and NSI (XRFS) soil data is given at the [BGS project web page](#) and enquiries should be sent to [enquiries@bgs.ac.uk](mailto:enquiries@bgs.ac.uk).

Other data sets providing information on soil chemistry are summarised in Appendix 2 of Ander *et al.* (2011) and this includes contact and web site links.

##### Soil parent material

The BGS Soil-Parent Material Model is described on a BGS web page ([SPPM](#))<sup>5</sup> and this contains information regarding further information and pricing.

##### Land use data including metalliferous mining and mineralisation

The Generalised Land Use Database (GLUD) Statistics for England 2005 is available for free from the [Communities and Local Government website](#).<sup>6</sup> Users interested in the detailed maps at land parcel level who hold the appropriate public sector licence to use OS MasterMap® can request to see the GLUD data at this large scale level ([gis@communities.gsi.gov.uk](mailto:gis@communities.gsi.gov.uk)).

The Ove Arup Mineralisation and mines data updated and modified by BGS is available from BGS subject to terms and conditions (see the [BGS project web page](#)).

<sup>4</sup> <http://www.bgs.ac.uk/gbase/NBCDefraProject.html>

<sup>5</sup> <http://www.bgs.ac.uk/products/onshore/soilPMM.html>

<sup>6</sup> <http://www.communities.gov.uk/publications/planningandbuilding/generalisedlanduse>

## Further Reading

The following is a list of bibliographic references that provide more detailed information regarding the distribution and behaviour of nickel in the surface environment. Some of these references are referred to in this supplementary information section.

Ander, E.L., Cave, M.R., Johnson, C.C. and Palumbo-Roe, B. 2011. Normal background concentrations of contaminants in the soils of England. Available data and data exploration. *British Geological Survey Commissioned Report*, CR/11/145. 124pp.

Ander, E.L., Breward, N., Flight, D.M.A., Lister, T.R., Smyth, D. and Young, M.E. In Press. Regional Geochemistry of Northern Ireland: environmental and health implications. *Geochemistry: Exploration-Environment-Analysis*.

Ander, E.L., Cave, M.R., Johnson, C.C. and Palumbo-Roe, B. 2012. Normal background concentrations of contaminants in the soils of England. Results of the data exploration for Cu, Ni, Cd and Hg. *British Geological Survey Commissioned Report*, CR/12/041. 88pp.

Appleton, J.D., Rawlins, B.G. and Thornton, I. 2008. National-scale estimation of potentially harmful element ambient background concentrations in topsoil using parent material classified soil:stream-sediment relationships. *Applied Geochemistry*, 23(9), 2596-2611.

Archer, F.C. and Hodgson, I.H. 1987. Total and extractable trace element contents of soils in England and Wales. *Journal of Soil Science*, 38, 421-431.

Bevins, R.E., Young, B., Mason, J.S., Manning, D.A.C. and Symes, R.F. (2010), *Mineralization of England and Wales*, Geological Conservation Review Series, No. 36, Joint Nature Conservation Committee, Peterborough, 598 pages, illustrations, A4 hardback, ISBN 978 1 86107 566 6. Available on-line at: <http://www.jncc.gov.uk/page-3298>. Last access 10th June 2012.

BGS. 1992. Regional geochemistry of the Lake District and adjacent areas. British Geological Survey Regional Geochemistry Atlas Series. BGS, Keyworth, Nottingham, UK. ISBN 0 85272 225 7.

BGS. 1996. Regional geochemistry of north-east England. British Geological Survey Regional Geochemistry Atlas Series. BGS, Keyworth, Nottingham, UK. ISBN 0 85272 255 9.

BGS. 1998. Minerals in Britain. Past production ... Future potential: Nickel and Platinum. A British Geological Survey Report for the Department of Trade and Industry, UK. Available on-line at: <http://www.bgs.ac.uk/downloads/start.cfm?id=1323>. Last access 10<sup>th</sup> June 2012.

Canadian Council of Ministers of the Environment. 1999. Canadian soil quality control guidelines for the protection of environmental and human health: Nickel. In: *Canadian environmental quality guidelines*, 1999, Canadian Council of Ministers of the Environment.

Cave, M.R., Johnson, C.C., Ander, E.L. and Palumbo-Roe, B. 2012. Methodology for the determination of normal background contaminant concentrations in English soils. *British Geological Survey Commissioned Report*, CR/12/003. 56pp.

Darnley, A.G., Bjorklund, A., Bolviken, B., Gustavsson, N., Koval, P.V., Plant, J.A., Steenfelt, A., Tauchid, M. and Xuejing, X. 1995. A global geochemical database for environmental and resource management. *UNESCO publishing*, 19.

Echevarria, G., Massoura, S.T., Sterckeman, T., Becquer, T., Schwartz, C. and Morel, J.L. 2006. Assessment and Control of the Bioavailability of Nickel in Soils. *Environmental Toxicology and Chemistry*, 25(3), 643-651.

Fordyce, F.M., Brown, S.E., Ander, E.L., Rawlins, B.G., O'Donnell, K.E., Lister, T.R., Breward, N. and Johnson, C.C. 2005. GSUE: Urban geochemical mapping in Great Britain: *Geochemistry: Exploration-Environment-Analysis*, 5(4), 325-336.

Johnson, C.C., Breward, N., Ander, E.L. and Ault, L. 2005. G-BASE: Baseline geochemical mapping of Great Britain and Northern Ireland. *Geochemistry: Exploration, Environment, Analysis*, 5(4), 347-357.

Johnson, C.C., Ander, E.L., Cave, M.R. and Palumbo-Roe, B. 2012. Normal Background Concentrations of contaminants in English soil: Final project report. *British Geological Survey Commissioned Report*, CR/12/035. 40pp.

### Supplementary Information

- Kierczak, J., Neel, C., Bril, H. and Puziewicz, J. 2007. Effect of Mineralogy and Pedoclimatic Variations on Ni and Cr Distribution in Serpentine Soils Under Temperate Climate. *Geoderma*, 142(1–2), 165-177.
- Lark, R.M. 2012. Some considerations on aggregate sample supports for soil inventory and monitoring. *European Journal of Soil Science*, February 2012, 63, 86-95.
- Lark, R.M., Bellamy, P.H. and Rawlins, B.G. 2006. Spatio-Temporal Variability of Some Metal Concentrations in the Soil of Eastern England, and Implications for Soil Monitoring. *Geoderma*, 133(3–4), 363-379.
- Lawley, R. 2011. The Soil-Parent Material Database: A User Guide. *British Geological Survey Open Report*, OR/08/034. 53pp. Available on-line from [NORA](#).
- Matheron, G. 1962. *Traité de géostatistique appliquée*. Tome I, Editions Technip, Paris, 334pp.
- Martin, I., Morgan, H., Jones, C., Waterfall, E. and Jefferies, J. 2009. Soil Guideline Values for nickel in soil. Science Report SC050021/Nickel SGV. Environment Agency, May 2009. Available on-line: <http://www.environment-agency.gov.uk/static/documents/Research/SCHO0409BPWB-e-e.pdf> . Last accessed 10<sup>th</sup> June 2012.
- McGrath, S.P. and Loveland, P.J. 1992. The Soil Geochemical Atlas of England and Wales. Blackie Academic and Professional, Glasgow.
- Nicholson, F.A., Smith, S.R., Alloway B.J., Carlton-Smith, C. and Chambers, B.J. 2003. An Inventory of Heavy Metals Inputs to Agricultural Soils in England and Wales. *Science of The Total Environment*, 311(1–3), 205-219.
- Ove Arup (1990). Mining Instability in Britain. Unpublished reports by Ove Arup for the Department of the Environment (DoE), UK. Associated data sets modified by BGS into GIS format (see <http://www.bgs.ac.uk/gbase/NBCDefraProject.html>).
- Paterson, E., Towers, W., Bacon, J.R. and Jones, M. 2003. Background levels of contaminants in Scottish soils. The Macaulay Institute. *Final Contract Report to SEPA*, 60pp.
- Rawlins, B.G., McGrath, S.P., Scheib, A.J., Cave, M.R., Breward, N., Lister, T.R., Ingham, M., Gowing, C.J.B., and Carter, S. 2012. The Advanced Soil Geochemical Atlas of England and Wales. British Geological Survey, Keyworth, Nottingham. Published as an electronic book. Available on-line at: [www.bgs.ac.uk/gbase/advsoilatlasEVV.html](http://www.bgs.ac.uk/gbase/advsoilatlasEVV.html) last accessed 10<sup>th</sup> June 2012. Nickel, pages 122-125.
- Reimann, C., de Caritat, P., GEMAS Project Team and NGSa Project Team. 2012. New soil composition data for Europe and Australia: demonstrating comparability, identifying continental-scale processes and learning lessons for global geochemical mapping. *Science of The Total Environment*, 416, 239-252.
- Rooney, C.P., Zhao, F. and McGrath, S.P. 2007. Phytotoxicity of Nickel in a Range of European Soils: Influence of Soil Properties, Ni Solubility and Speciation. *Environmental Pollution*, 145(2) 596-605.
- Saikat, S., Barnes, B. and Westwood, D. 2007. A review of laboratory results for bioaccessibility values of arsenic, lead and nickel in contaminated UK soils. *Journal of Environmental Science and Health Part A*, Vol. 42, 1213 - 1221.
- Salminen, R. (chief ed.) et al. 2005. [Geochemical Atlas of Europe. Part I - Background Information, Methodology and Maps](#). Geological Survey of Finland, Otamedia Oy, Espoo, 525 pp.
- Sanders, J.R., McGrath, S.P. and Adams, T.McM. 1987. Zinc, Copper and Nickel Concentrations in Soil Extracts and Crops Grown on Four Soils Treated with Metal-Loaded Sewage Sludges. *Environmental Pollution*, 44 (3), 193-210.
- Smyth, D. 2007. Methods used in the Tellus Geochemical Mapping of Northern Ireland. British Geological Survey Open Report OR/07/022. 89pp. Available on-line from [NORA](#) last accessed 1<sup>st</sup> May 2012.
- Spurgeon, D.J., Rowland, P., Ainsworth, G., Rothery, P., Long, S. and Black, H.I.J. 2008. Geographical and Pedological Drivers of Distribution and Risks to Soil Fauna of Seven Metals (Cd, Cu, Cr, Ni, Pb, V and Zn) in British Soils. *Environmental Pollution*, 153(2), 273-283.
- Tye, A.M., Young, S., Crout, N.M.J., Zhang, H., Preston, S., Zhao, F.J., McGrath, S.P. 2004. Speciation and solubility of Cu, Ni and Pb in contaminated soils. *European Journal of Soil Science*, 55, 579-590.

Webb, J.S, Thornton, I, Thompson, M, Howarth, R.J, and Lowenstein, P.L. 1978. *The Wolfson geochemical atlas of England and Wales*. Clarendon Press, Oxford.